Machine Learning

Support Vector Machines

(contains material adapted from talks by Constantin F. Aliferis & Ioannis Tsamardinos, and Martin Law)

Support Vector Machines

- Are binary classifiers
- Are very popular because
  - They are very effective classifiers in many domains
  - They can train fairly quickly on large data sets
  - They can be used without understanding their underlying math
  - …yet those who want to can geek out on the formulae.

Support Vector Machines

Main ideas:

1. Find an "optimal" hyperplane to split the data into two sets: <u>maximize margin</u>

2. Extend the above definition for non-linearly separable problems: <u>have a penalty term for misclassifications</u>

3. Map data to high dimensional space where it is easier to classify with linear decision surfaces: <u>reformulate problem so that data is mapped implicitly to this space</u>

Defining a hyperplane

- Any hyperplane can be written as the set of points $\mathbf{x}$ satisfying the equation below, where $\boldsymbol{w}$ and $\boldsymbol{x}$ are vectors in $\mathbf{R}^{\mathbf{d}}$

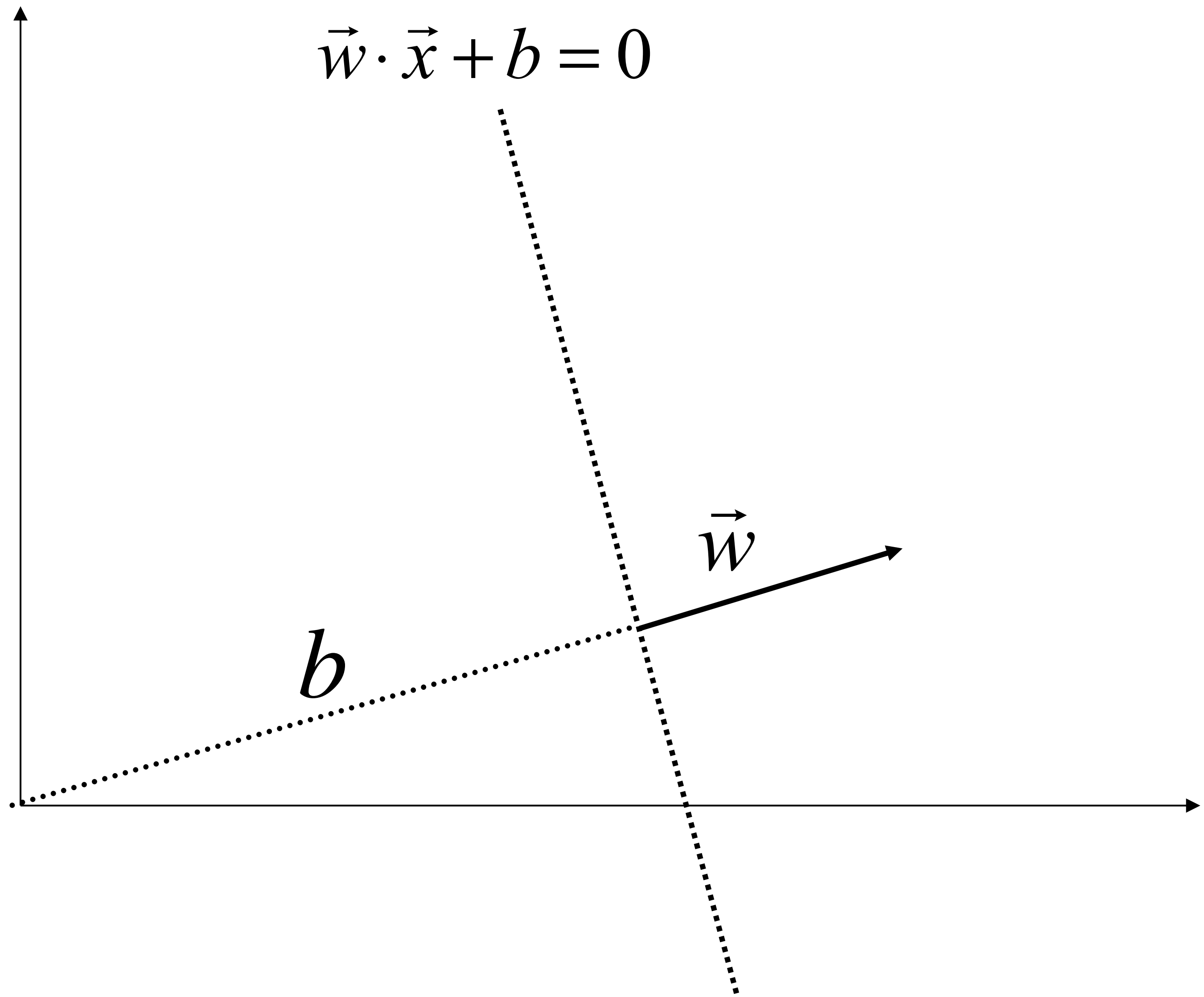
$$w \cdot x + b = 0$$

- The vector **w** is a normal vector: it is perpendicular to the hyperplane. The parameter *b* determines the offset of the hyperplane from the origin along the normal vector.

Euclidean norm

$$\text{dist to origin} = \frac{|b|}{\|w\|}$$

A hyperplane in 2 dimensions



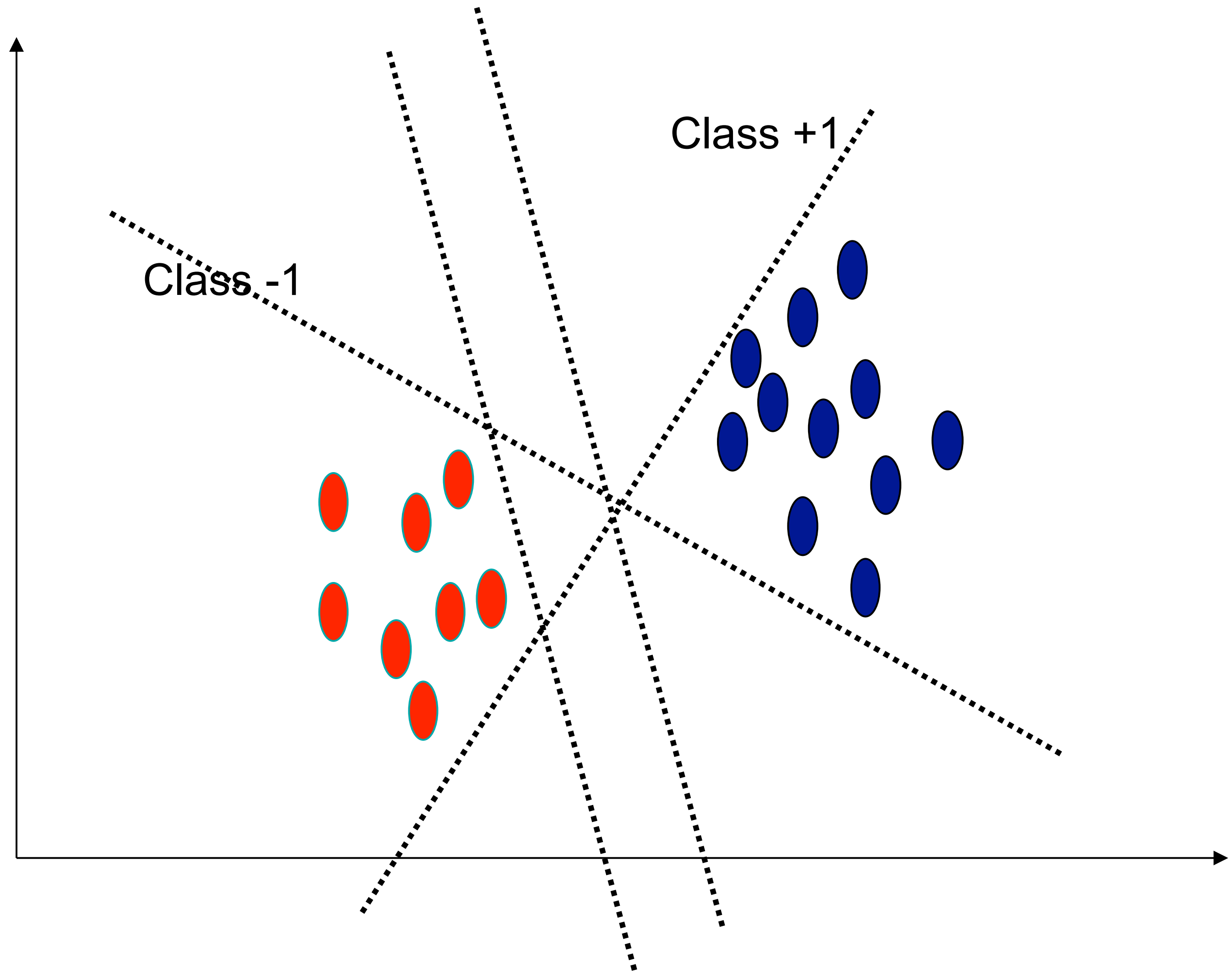
Some definitions

- Assume training data consisting of vectors of *d* real values that belong to class 1 or class -1

$$D = \{(x_i, y_i) \mid x_i \in \Re^d, y_i \in \{-1,1\}\}$$

- Find a hyperplane to separate the data into the two classes (assume this is possible, for the moment).

Which hyperplane is best?



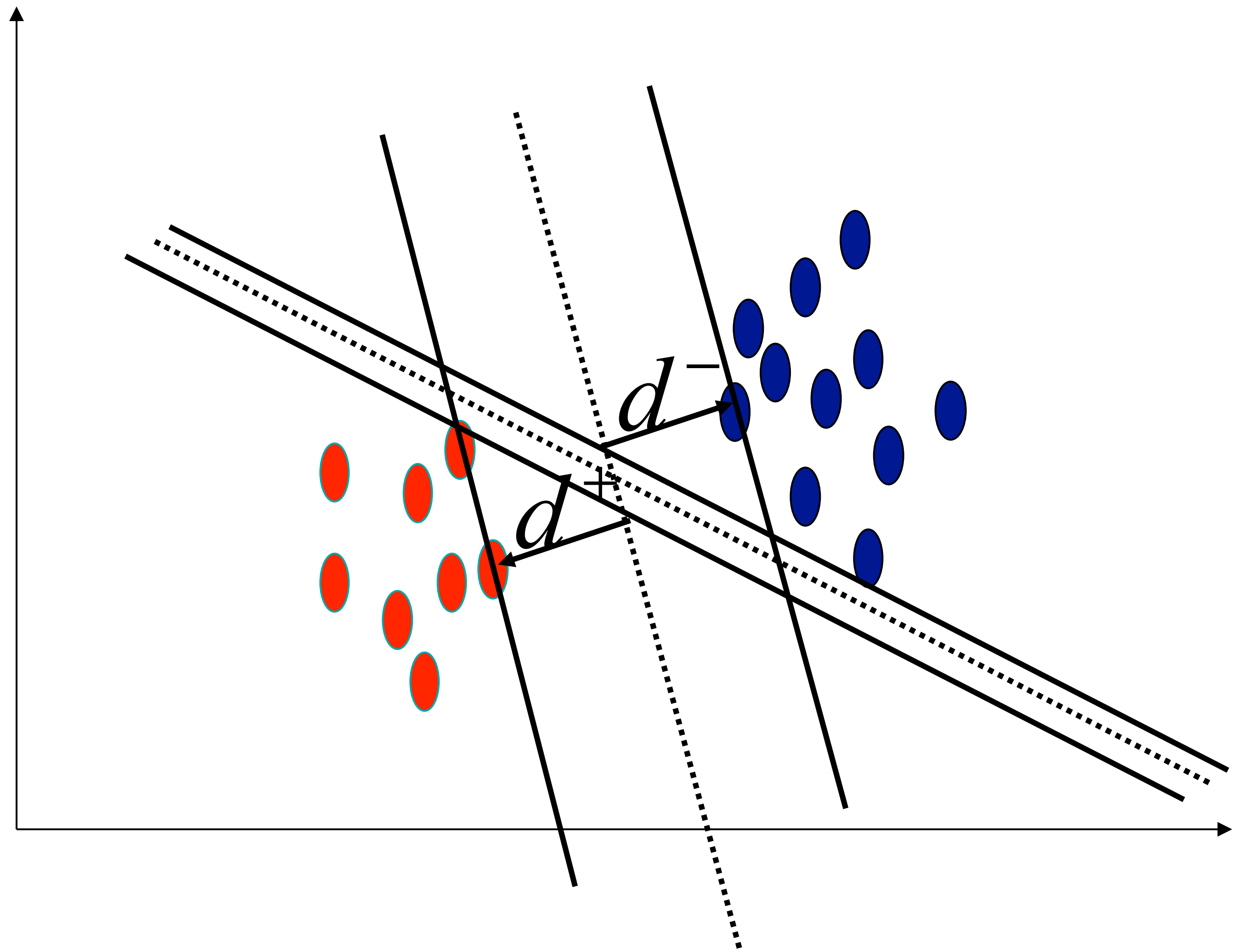
The margin

- Define d+ as the distance from a hyperplane to the closest positive example.
- Define d- as the distance to the closest negative example
- Define the “margin”, m as…

$$m = d^+ + d^-$$

- Look for the largest margin!

An example



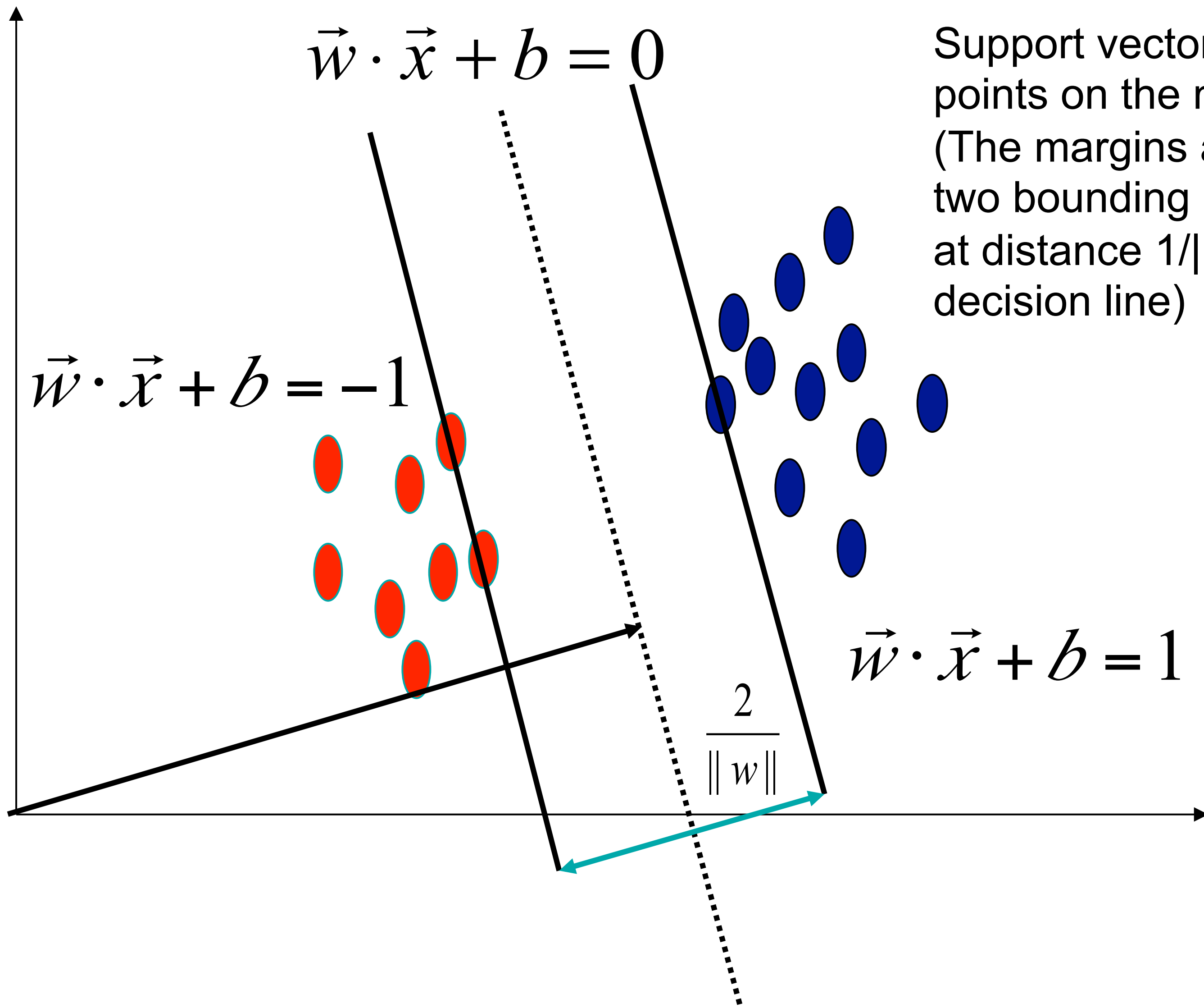
The margin

- There is some scale for **w** and for b where the following equation holds.

$$d^{+} = d^{-} = \frac{1}{\| w \|}$$

- Those data points that lie within distance 1/||w|| of the hyperplane are called the **support vectors.**
- The support vectors define two planes parallel to the hyperplane separator

Three hyperplanes to consider



Support vectors are points on the margins (The margins are the two bounding hyperplanes at distance 1/||w|| from the decision line)

Optimization = maximize margin

- We write the optimization problem as…

$$\text{maximize}\left(\frac{2}{\|w\|}\right)$$

$$\text{such that } y_i(w \cdot x_i + b) \geq 1, \forall \{x_i, y_i\} \in D$$

remember y_i is the class label, and $y_i \in \{-1, 1\}$

Maximizing margins (not mathy)

- Given a guess of **w** and b we can…
  - See if all data points are correctly classified
  - Compute the width of the margin

- Now, we just search the space of **w**'s and b's to find the widest margin hyperplane that correctly classifies the data.

- How?

  Gradient descent? Simulated Annealing?

  Matrix Inversion?

A little more mathy

Find **w** and *b* to maximize

$$\text{margin} = \frac{2}{\|\mathbf{w}\|}$$

$$\text{such that } y_i(w \cdot x_i + b) \geq 1, \forall \{x_i, y_i\} \in D$$

- This is a quadratic function with linear constraints.
- Quadratic optimization problems have known algorithmic solutions.
- Naively, this quadratic optimization can be solved in O(n^3) time, where n = the number of data points.

Still mathy-er

- Maximizing $\left(\frac{2}{\|w\|}\right)$ equivalent to minimizing $\|w\|$
- For math convenience we ACTUALLY minimize

$$\frac{1}{2}\|w\|^2$$

- Now, we associate a Lagrange multiplier α_i with each point x_i in the data. This gives…

$$L_p \equiv \frac{1}{2}\|w\|^2 - \sum_{i=1}^{|D|} \alpha_i y_i (x_i \cdot w + b) + \sum_{i=1}^{|D|} \alpha_i$$

(psst: What's a Lagrange Multiplier?)

- A way of optimizing a function subject to one (or more) constraint(s) from another function(s).

- You incorporate the original function and the constraint equations into one new equation and then solve.

- For more, check out the wikipedia.

Why use Lagrangian Multipliers?

- We want to put a line between the sets that maximize the margin between classes subject to the constraint all points are correctly classified.
- So…

  The margin maximization is a classic maximization problem

  Classifying each point correctly is a constraint
- This is exactly the setup needed for Lagrangians

The Lagrangian “dual”

- In practice, people don’t minimize this formula from the previous slide.

$$L_p \equiv \frac{1}{2}\| w \|^2 - \sum_{i=1}^{|D|} \alpha_i y_i (x_i \cdot w + b) + \sum_{i=1}^{|D|} \alpha_i$$

- Instead they maximize its “dual,” which will also give us what we need and is in a more convenient format for later work.

$$L_D \equiv \sum_{i=1}^{|D|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|D|} \sum_{j=1}^{|D|} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j)$$

The Lagrangian "dual"

- When we maximize this, a cool thing happens. Only those points defining the margin have non-zero values for α

$$L_D \equiv \sum_{i=1}^{|D|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|D|} \sum_{j=1}^{|D|} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j)$$

- Note also this formulation relates two examples to each other via a dot product.
- This will become meaningful later…

Classification with SVM

- For testing, the new data **z** is classified as class 1 if $f \geq 0$ and as class -1 if $f < 0$

- SO…our weights are determined by this (where S is the number of support vectors)

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

- And our decision function is a normal linear discriminant.

$$f = \mathbf{w}^T \mathbf{z} + b$$

Classification with SVM: PART 2

While our decision function is a normal linear discriminant….

$$f = \mathbf{w}^T\mathbf{z} + b$$

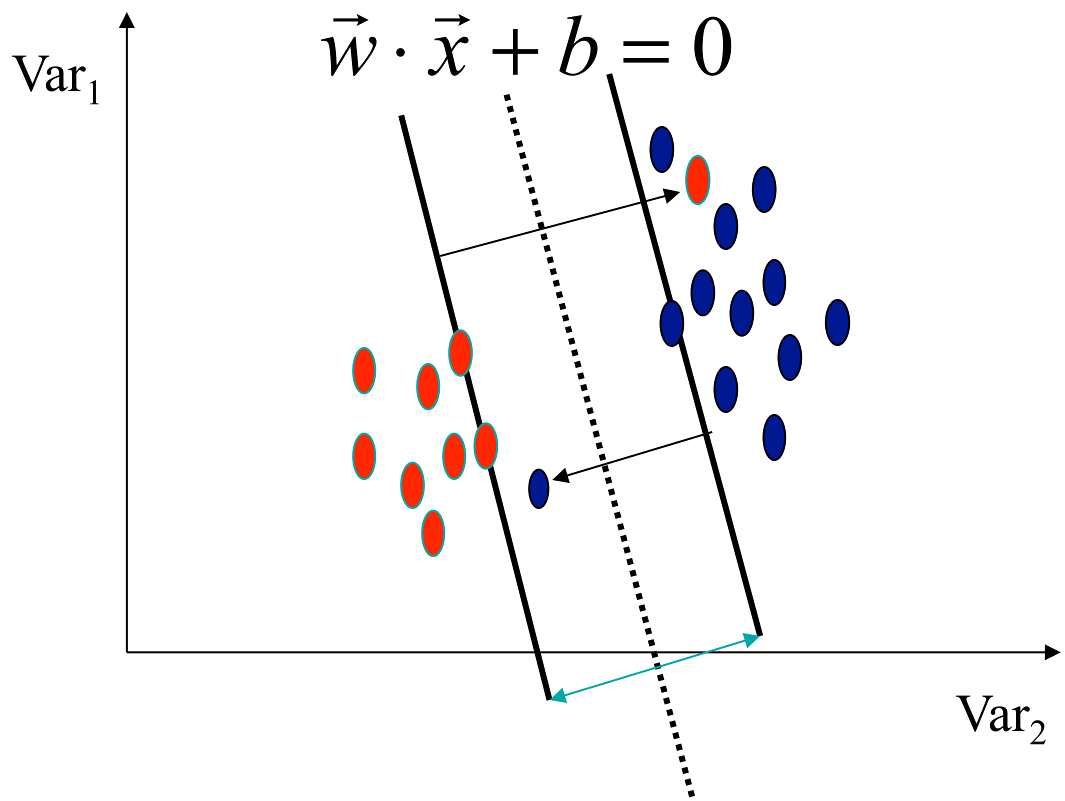
…people usually calculate the class using the support vectors (those data points with non-0 alpha values that lie on the +1 and -1 margins).

$$f = \mathbf{w}^T\mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}^T \mathbf{z} + b$$

The new element z is compared to all the support vectors and its value is determined by where it lies in comparison to them.

What if we have noisy training data?

- Can we combine minimizing misclassifications (with some forgiveness) with maximizing the margin?



Support Vector Machines

Main ideas:

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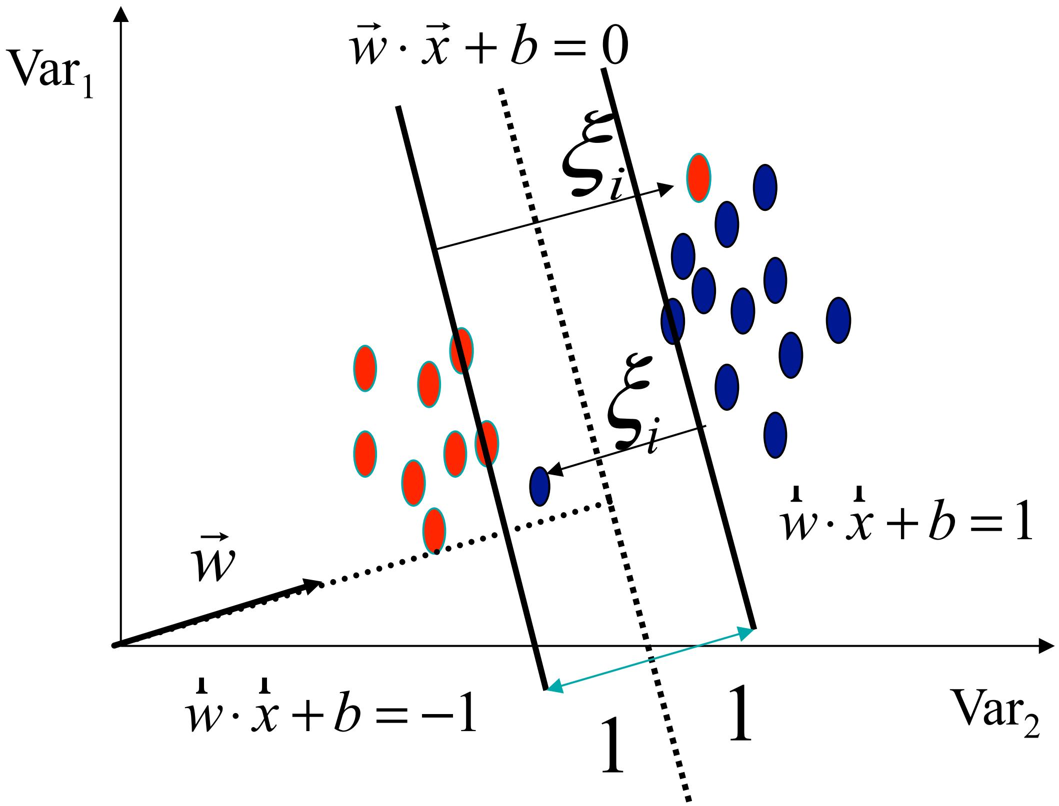
2. Extend the above definition for non-linearly separable problems: <u>have a penalty term for misclassifications</u>

3. Map data to high dimensional space where it is easier to classify with linear decision surfaces: <u>reformulate problem so that data is mapped implicitly to this space</u>

Non-Linearly Separable Data



Allow some instances to fall within the margin, but penalize them

Introduce slack variables ξ_i (one per data point)

The constraints then become…

$$y_i(w \cdot x + b) \geq 1 - \xi_i \quad \forall (x_i, y_i) \in D, \xi_i \geq 0$$

Formulating the Problem

- We are now minimizing this formula

$$\frac{1}{2} w \cdot w + C \sum_i \xi_i$$

- Subject to the constraints

$$y_i (w \cdot x + b) \geq 1 - \xi_i \quad \forall (x_i, y_i) \in D, \xi_i \geq 0$$

- Where C determines the weight to give misclassification error.

Linear, Soft-Margin SVMs

$$\min \frac{1}{2}\|w\|^2 + C\sum_i \xi_i \qquad \begin{aligned} & y_i(w \cdot x_i + b) \geq 1 - \xi_i,\ \forall x_i \\ & \xi_i \geq 0 \end{aligned}$$

- Algorithm tries to minimize ξ_i while maximizing margin
- Notice: algorithm does not minimize the *number* of misclassifications, but the sum of distances from the margin hyperplanes
- As $C \to \infty$, we get closer to the hard-margin solution

The Lagrange Dual

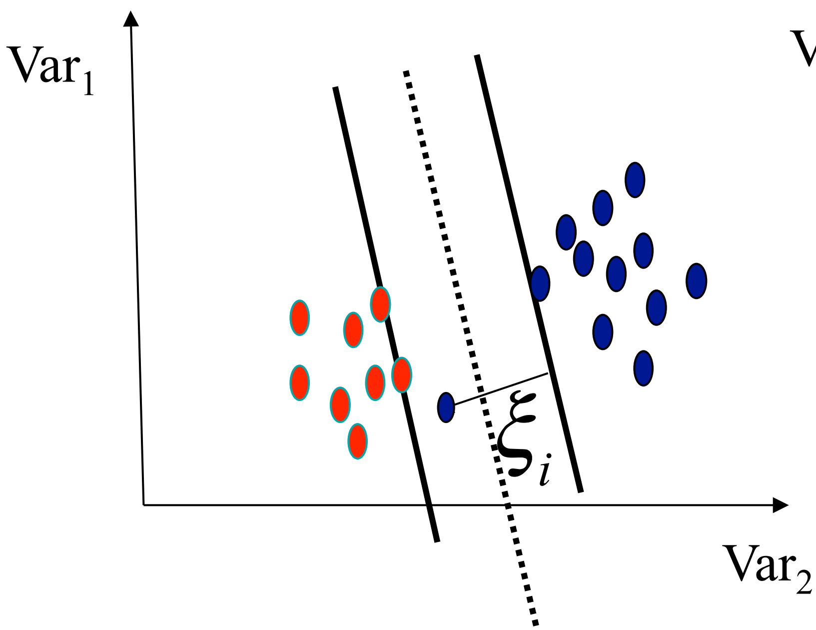
- The dual of the "soft" problem is

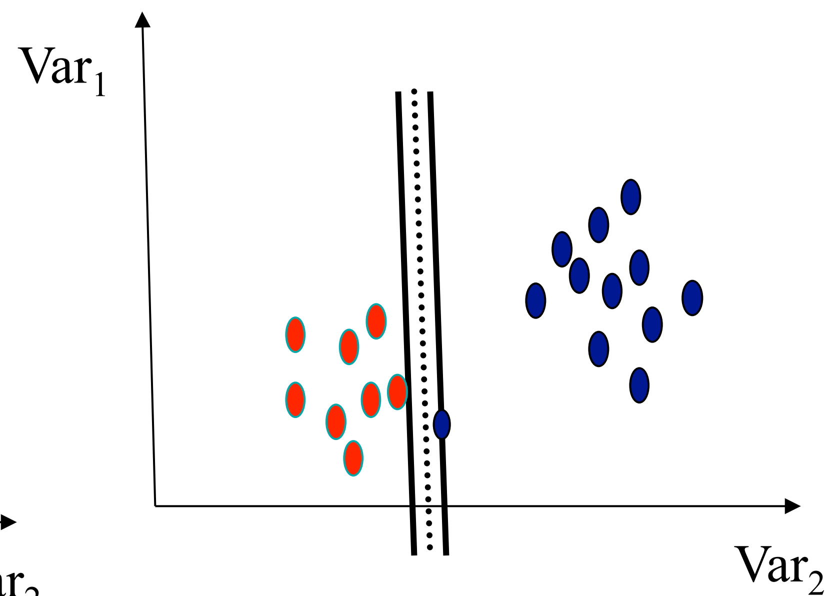
$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- **w** is also recovered as $\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$
- The only difference with the linearly separable case is that there is an upper bound *C* on α_i
- Once again, a QP solver can be used to find α_i

Robustness of Soft vs Hard Margin





Soft Margin SVM

Hard Margin SVM

Soft vs Hard Margin SVM

- Soft-Margin always have a solution
- Soft-Margin is more robust to outliers
  - Smoother surfaces (in the non-linear case)
- Hard-Margin requires no parameters at all

Linear SVMs: Overview

- The classifier is a *separating hyperplane.*
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers.
- Both in the dual formulation of the problem and in the solution, training points appear only inside inner products:

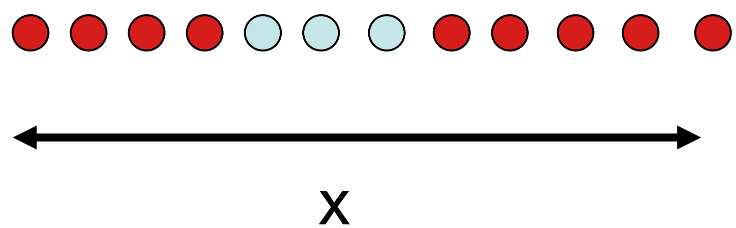
$$L_D \equiv \sum_{i=1}^{|D|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|D|} \sum_{j=1}^{|D|} \alpha_i \alpha_j y_i y_j \boxed{(x_i \cdot x_j)}$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

Extension to Non-linear Decision Boundary

- So far, we have only considered large-margin classifier with a linear decision boundary
- What if the decision boundary is non-linear?

A one-dimensional decision problem



Support Vector Machines

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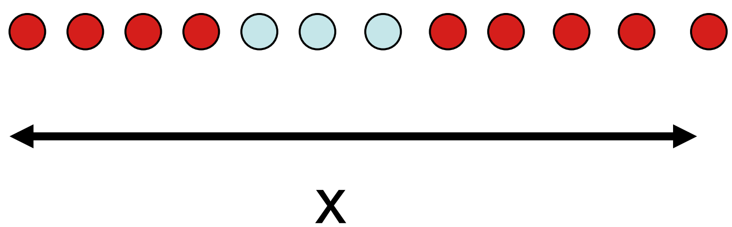
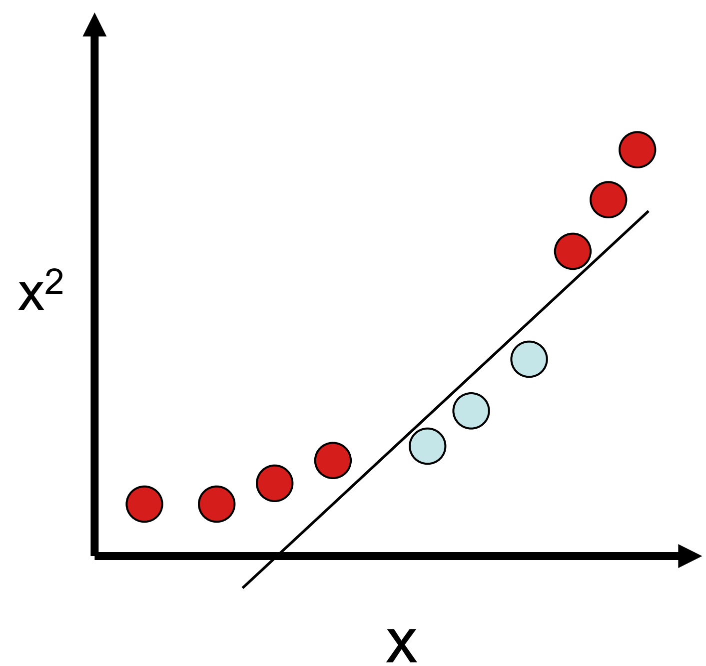
Higher dimensional mapping

- The idea is to map the vectors to a higher dimensional space to gain linear separation.

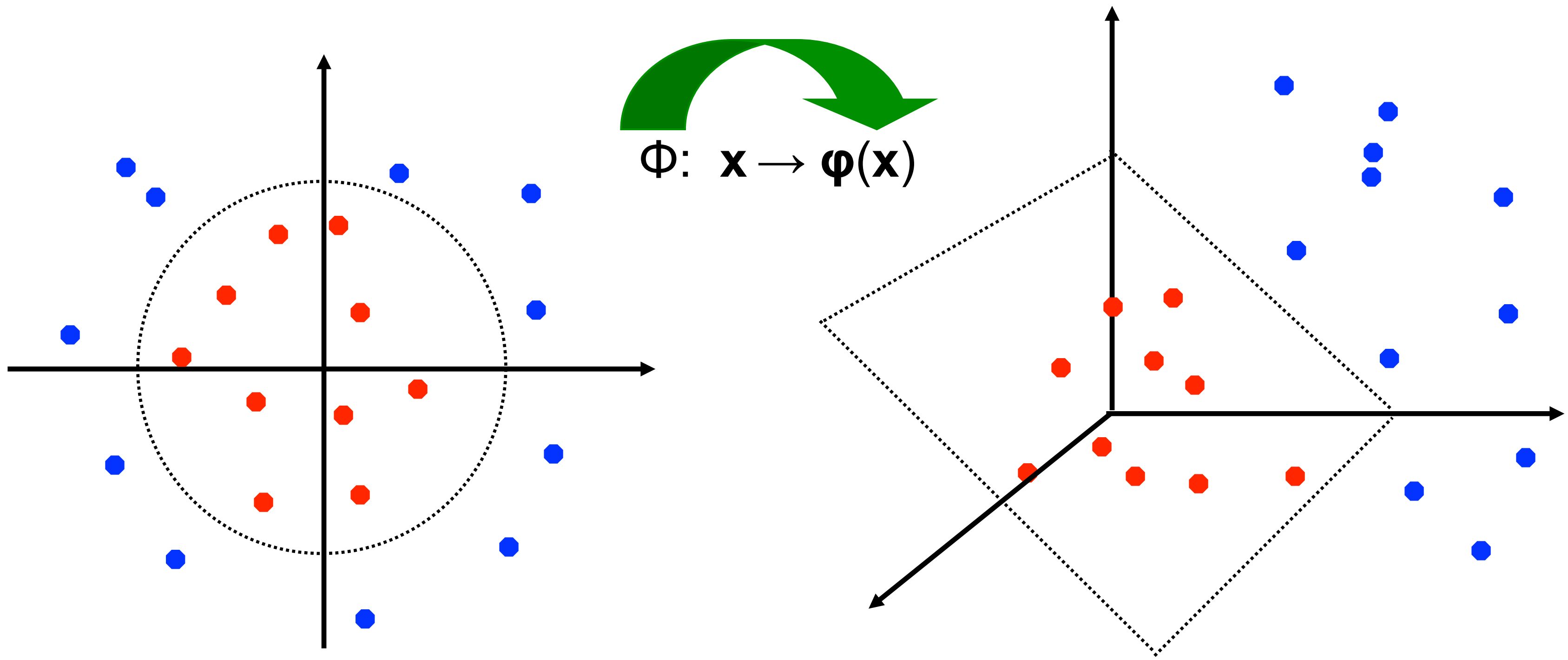




Mapping x onto $\{x^2,x\}$ gives linear separation.

Non-linear SVMs: Feature spaces

- General idea: the original feature space can be mapped to some higher-dimensional feature space where the training set is separable:



What this does to the math

- Recall the SVM optimization problem with its inner product between data points

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- If we transform the data into a new vector space, this changes the math ever so slightly to be…

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

What are Kernel Functions

$$K(x_1, x_2) = \left\langle \Phi(x_1), \Phi(x_2) \right\rangle$$

- Kernels are functions that return inner products between the images of data points
- Since they are inner products, they can be thought of as similarity functions

Why Use Kernel Functions

$$K(x_1, x_2) = \left\langle \Phi(x_1), \Phi(x_2) \right\rangle$$

- You can define kernels for many things that aren't vectors of real values in Euclidean space (e.g. text documents)
- As long as we can calculate the inner product in the original feature space, we do not need to explicitly calculate the mapping Φ
- It can often be more efficient to compute K directly, without going through the step of computing Φ

That math again…

This original formula…

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

…becomes this, when we apply a data transformation…

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

…and if we can define a kernel…

$$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

…it becomes this…

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

An Example Kernel

- Suppose ϕ is given as follows

$$\phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

- An inner product in the feature space is

$$\langle \phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}), \phi(\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}) \rangle = (1 + x_1y_1 + x_2y_2)^2$$

** NOTE: On this slide *y* is not the label, it is a feature vector, just like *x* **

- So, if we define the kernel function as follows, there is no need to carry out f(.) explicitly

$$K(\mathbf{x}, \mathbf{y}) = (1 + x_1y_1 + x_2y_2)^2$$

- This use of kernel function to avoid calculating ϕ explicitly is known as the **kernel trick**

Examples of Kernel Functions

** NOTE: On this slide *y* is not the label, it is a feature vector, just like *x* **

- Polynomial kernel with degree *d*

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y}+1)^d$$

- Radial basis function kernel with width s

$$K(\mathbf{x},\mathbf{y}) = \exp(-||\mathbf{x}-\mathbf{y}||^2/(2\sigma^2))$$

  - Closely related to radial basis function neural networks
  - The feature space is infinite-dimensional
- Sigmoid with parameter k and q

$$K(\mathbf{x},\mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y}+\theta)$$

  - It does not satisfy the Mercer condition on all k and q

Building Kernels from Other Kernels

- Kernels can be composed from other kernels
- The following 2 slides give some basic rules for building complex kernels from simple kernels

Definitions for the following slide

$k_1(x,x')$ and $k_2(x,x')$ are valid kernels on $\{\mathrm{x},\mathrm{x}'\} \in S$

S is some set (of anything: emails, images, integers)

$c > 0$ is a constant

$f(\cdot)$ is any function

$q(\cdot)$ is a polynomial with non-negative coefficients

$\phi(\mathrm{x})$ is a function from the -> $\mathbb{R}^m$

$k_3(\cdot,\cdot)$ is a valid kernel in $\mathbb{R}^m$

A is a symmetric positive semidefinite matrix

$x = (x_a, x_b)$ ....essentially, x can be decomposed into subparts

...like scalars in a vector

$k_a(\cdot,\cdot), k_b(\cdot,\cdot)$ are valid kernels over their respective spaces

Techniques for Kernel Construction

Given valid kernels $k_1(x,x')$ and $k_2(x,x')$,

the following are also valid kernels

$$k(x,x') = ck_1(x,x')$$

$$k(x,x') = f(x)k_1(x,x')f(x')$$

$$k(x,x') = q(k_1(x,x'))$$

$$k(x,x') = \exp(k_1(x,x'))$$

$$k(x,x') = k_1(x,x') + k_2(x,x')$$

$$k(x,x') = k_3(\phi(x),\phi(x'))$$

$k(x,x') = x^T A x'$ This one assumes x,x' are vectors

$$k(x,x') = k_a(x_a,x'_a) + k_b(x_b,x'_b)$$

$$k(x,x') = k_a(x_a,x'_a)k_b(x_b,x'_b)$$

Classifying with a Kernel

- For testing, the new data **z** is classified as class 1 if $f \geq 0$ and as class -1 if $f < 0$

Original

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

$$f = \mathbf{w}^T \mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}^T \mathbf{z} + b$$

With kernel function

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \phi(\mathbf{x}_{t_j})$$

$$f = \langle \mathbf{w}, \phi(\mathbf{z}) \rangle + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

NOTE: ***y*** is once again a label from the set {-1, 1} **

Strengths and Weaknesses of SVM

- Strengths
  - Training is relatively easy
    - No local maximum, unlike in neural networks
  - It scales relatively well to high dimensional data
  - Tradeoff between classifier complexity and error can be controlled explicitly
  - Non-traditional data like strings and trees can be used as input to SVM, instead of feature vectors
- Weaknesses
  - Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner.

You as the SVM user

- You have two main choices to make:
  1) What kernel will you use?

     Polynomial?

     Radial Basis Function?

     Something else?

  2) How much "slack" will you allow?

     Depends on how much you trust data collection and labeling.

SVM applications

- SVMs were originally proposed by Boser, Guyon and Vapnik in 1992 and gained increasing popularity in late 1990s.
- SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
- SVM techniques have been extended to a number of tasks such as regression [Vapnik *et al.* '97], principal component analysis [Schölkopf *et al.* '99], etc.
- Most popular optimization algorithms for SVMs use *decomposition* to hill-climb over a subset of a_i's at a time, e.g. SMO [Platt '99] and [Joachims '99]